

Physical Chemistry
ALANINE SOLVATION.

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Ab initio study of the addition of successive water molecules to the amino acid L-alanine in both neutral and zwitterion form. Focused on the number of water molecules needed to stabilize the zwitterion form, and how the solvent effects conformational preference. The solvent is modeled by ab initio, EFP (Effective Fragment Potential), and the isotropic dielectrics PCM (Polarizable Continuum Method) bulk solvation techniques. The study is undertaken at the RHF (Restricted Hartree Fock) and 6N31++** with the GAMESS (General Atomic and Molecular Electronic Structure System).